Quantum Computing in Practice: A Multilayer Embedding Approach for Near Future Applications

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Quantum computers are special purpose machines that are expected to be particularly useful in simulating strongly correlated chemical systems. The quantum computer excels at treating a moderate number of orbitals within an active space in a fully quantum mechanical manner. To illustrate this, a quantum phase estimation calculation on F_2 in a (2,2) active space is presented. While this is a promising start, it also underlines the need for carefully selecting the orbital spaces treated by the quantum computer. To this end, a scheme for selecting such an active space semi-automatically is described and simulated results obtained using both the quantum phase estimation (QPE) and variational quantum eigensolver (VQE) algorithms are presented and combined with a subtractive method to enable accurate description of the environment. The active occupied space is selected from orbitals localized on the chemically relevant fragment of the molecule, while the corresponding virtual space is chosen based on the magnitude of interactions with the occupied space calculated from perturbation theory. This protocol is then applied to two chemical systems of biological/pharmaceutical relevance: the enzyme [Fe] hydrogenase and the photosenzitizer temoporfin. While the sizes of the active spaces currently amenable to a quantum computational treatment are not enough to demonstrate quantum advantage, the procedure outlined here is applicable to any active space size, including those that are outside the reach of classical computation.